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2015 J. Phys.: Conf. Ser. 635 072020

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Potential electron scattering by the phosphorous systems P_n ($n = 1 \div 3$)

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Synopsis Independent atom model and the optical potential approach are used in order to calculate the differential and integral cross sections for the electron scattering by single-, two- and three-atom compounds of phosphorus. The potentials and atomic characteristics are determined in the local approach of the stationary and time-dependent density functional theory with account of some relativistic effects for the corresponding study of electron scattering process on the atoms from the molecules.

We have used the optical potential approach [1,2] for the $e+P_n$ ($n=1 \div 3$) elastic scattering in the independent atom model (IAM) [3,4] for the cross section calculations. The static-exchange approximation in the SMC method were used with pseudopotentials in [5] for the calculation of integral (ICSs) and differential cross sections (DCSs) of electron scattering by X_2 and XH_3 molecules ($X=N, P, As$).

The DCSs of potential electron scattering by an N -atomic molecule in the IAM is given [3,4]

$$\frac{d\sigma_{el}}{d\Omega} = \sum_{m=1}^N \sum_{n=1}^N [f_m(\theta, k) f_n^*(\theta, k) + g_m(\theta, k) g_n^*(\theta, k)] \frac{\sin(sr_{mn})}{sr_{mn}}$$

Here f_m , g_m are the scattering angle, the direct and spin-flip amplitudes due to the m -th atom of the molecule; θ ; while $k = \sqrt{2E}$, where E

is the electron energy; r_{mn} is the distance between the n -th and m -th atoms (calculated by the GAMESS code). Elastic, momentum transfer and viscosity ICSs are calculated from the DCSs by integration along the scattering angle.

We have used the local relativistic parameter-free real optical potential approximation (RSEPLA). It contains static, local exchange, polarization (local correlation-polarization), scalar-relativistic and spin-orbit potentials [1,2].

Polarization potential at large distances has an asymptotic form $-\alpha_d(0)/2r^4$, where $\alpha_d(0)$ – dipole static polarizability of the n -th atom calculated in the local approximation of time-dependent density functional theory (for the P atom it is $30.65 a_0^3$).

The cross sections are calculated in the 0.5÷30 eV energy region. On the Fig.1, as an example, we present the DCSs at 10 eV of impact energy. At all other impact energies E atomic and molecular DCSs have a similar special form. At small ($<60^\circ$) and large ($>150^\circ$) angles the DCSs [5] are close to our calculated atomic DCS while at intermediate angles they are between our DCSs for $e+P$ and $e+P_2$. On the Fig.2 the elastic ICSs are presented. A similar behavior of the momentum transfer and viscosity ICSs was obtained.

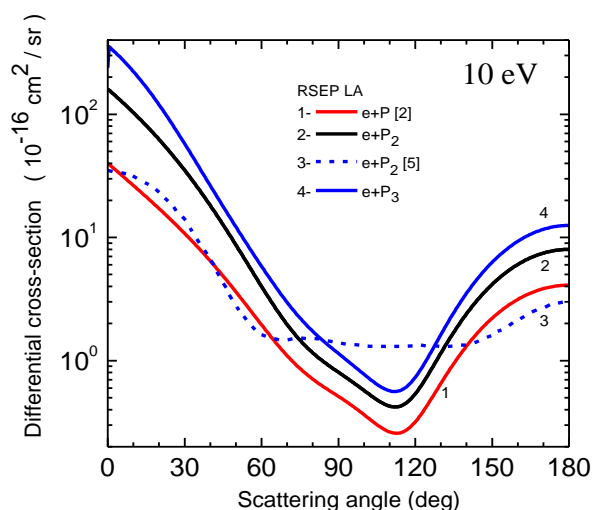


Figure 1. Differential cross sections at 10 eV.

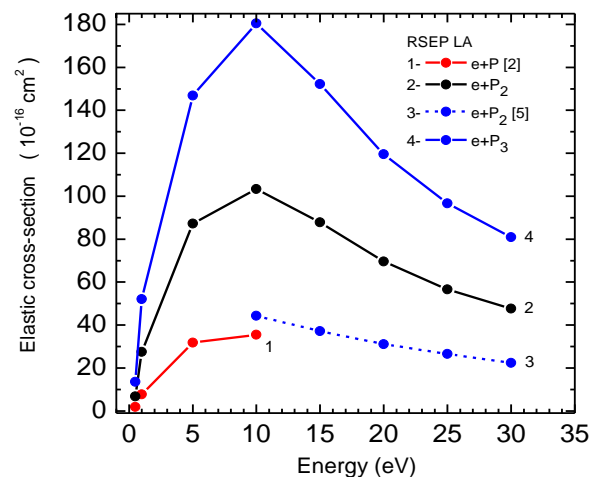


Figure 2. Elastic integral cross sections.

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